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Ice–ocean boundary conditions for coupled models

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Abstract

Coupled general circulation models are becoming more sophisticated, particularly with respect to the sea ice component and the increasing use of free surface formulations in the ocean. It is therefore timely to revisit the boundary conditions at the sea ice–ocean interface to ensure that (a) mass and energy are conserved, (b) the physics represented is as realistic as possible, and (c) numerical instabilities are avoided. We present here an overview of recent practice from the GISS, NCAR CCSM2.0 and MPI Hamburg coupled models. A new formulation of the basal sea ice fluxes, discussions of lateral melt and snow–ice formation, coupling strategies for the sea ice dynamics component, and interactions with dynamic free surfaces are presented.

Keywords: General circulation models; Sea ice thermodynamics; Sea ice dynamics; Ocean; Ice–ocean; Coupling; Artic

1. Introduction

There are a huge variety of physical environments that must be simulated in any comprehensive earth system model incorporating ocean, atmosphere, sea ice and land surface components. This implies that the models must work under a very wide range of conditions that sometimes are not central to the development of any single component model (such as the land surface or ocean). An extra burden for developers of coupled models occurs at the interfaces of different components

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(and scientific disciplines). Clearly defining what happens at these interfaces is also of paramount importance for improving interoperability or modularity of climate system components from different groups (a central focus in the ongoing PRogramme for Integrated earth System Modeling (PRISM) and Earth System Modeling Framework (ESMF) projects).

This paper addresses developments in coupling at sea ice–ocean interface. We do not attempt a complete review of current ice modeling practice, but we discuss our experience of the three models (National Center for Atmospheric Research (NCAR) Community Climate System Model (CCSM) 2.0, Goddard Institute for Space Studies (GISS) ModelE, and the Max-Planck-Institute für Meteorolgie (MPI) models) with which we are most familiar. Sea ice has historically been quite poorly represented in fully coupled models (relative to the sophistication of stand-alone ice, or ice–ocean models) (Randall et al., 1998). However, a greater appreciation for the role of sea ice processes in climate has led to significant improvements over recent years (Fichefet and Morales Maqueda, 1997; Bitz et al., 2001, amongst others). Additionally, development in ocean models has led to a widespread adoption of free surface formulations (as opposed to the rigid lid approximation) and the consequent use of so-called 'natural' boundary conditions (Griffies et al., 2000). The combination of these two advances has consequences for the coupling of the two components. For example, in going from a zero layer ice model (Semtner, 1976; Parkinson and Washington, 1979) to a multi-layer ice model with non-zero heat capacity, the conservation of energy at the interface becomes considerably more complex (Holland and Jenkins, 1999; Bitz and Lipscomb, 1999; Winton, 2000).

In order to satisfy demands for physically realistic boundary conditions and the need for improved interoperability of ocean and sea ice components, boundary conditions and fluxes should conform to two principles: (i) absolute conservation of mass, salt and energy, and (ii) as far as possible, no assumptions within the ocean or ice component can be made about the capabilities/approximations of the other component. Energy conservation should of course be fundamental and there are practical effects if it is not strictly enforced. For instance, if there are any erroneous energy sinks or sources associated with sea ice, variations in climate (and hence sea ice amount) will lead to systematic changes in the magnitude of such errors. This may provide a forcing comparable in size to an imposed forcing, for example, related to greenhouse gas concentrations. Even in a control run, any systematic offset between atmospheric surface fluxes and the fluxes into the ocean can cause increased drift in the deep ocean. Not all of the comments and recommendations discussed in this paper will lead to significant improvements of coupled simulations (compared to observations). However, most non-conservation issues can be dealt with very simply, and we believe that we should strive to get these fundamentals correct at all levels of approximation.

Whenever there is a transfer of mass from one component to another, the energy that is transferred depends on the energy reference level (ERL) (i.e. the temperature/phase at which the energy is defined to be zero). It is absolutely fundamental that each component knows what the relevant ERL is for any mass flux, and therefore it is convenient to use the same ERL for all mass fluxes between components of the model. In accord with common practice, for pure water we will use an ERL of liquid at 0 °C. For mixtures of salt and water, we use a similar ERL (i.e. energy is zero for the liquid + solute at 0 °C).

Given an ERL, we define the internal energy of ice E_i to be minus the energy required to bring the ice to the ERL (i.e. to melt it completely and warm to 0 °C). Depending on the assumptions made in the sea ice model, the formulation of this energy will differ. We will consider three possible cases: 1. pure ice (hereafter abbreviated as PI), 2. saline ice (but only with regard to the mass budget) (SI), and 3. saline ice with regard to both mass and energy budgets (i.e. with thermodynamically active brine pockets) (BP). In the latter case, brine pockets are explicitly parameterized to account for internal melting/freezing at the brine pocket-ice interface using an energy conserving formulation (following Bitz and Lipscomb, 1999 and references therein). Other formulations that attempt to include thermodynamic salinity effects without properly considering the expansion and contraction of brine pockets can lead to non-energy conserving schemes (for instance, the unmodified Maykut and Untersteiner (1971) or the 3-layer Semtner (1976) formulation), and we do not recommend their use in coupled models. For reference, the MPI model uses a zero-layer formulation (a version of PI that neglects the specific heat capacity of ice and snow) Semtner (1976), GISS modelE uses the SI formulation, while the latest NCAR CCSM2.0 uses the BP formulation (Briegleb et al., 2002). The modified Semtner 3-layer code derived by Winton (2000) uses the BP in the upper ice layer, and PI in the lower layer. Analytic ice models (such as used in Oberhuber (1993) or discussed by Leppäranta (1993)) are generally PI or zero-layer.

We define the energy per unit mass, rather than volume, since mass is the more fundamental quantity. For pure ice (PI), the (internal) energy of sea ice (J/kg) is

$$E_i = -L_0 + T_i c_i \tag{1}$$

where $L_0 = 3.34\times10^5$ J/kg is the latent heat of melting at 0 °C, T_i the temperature of the ice (in °C) and $c_i = 2060$ J/kg/°C is the specific heat of pure ice. For the SI case,

$$E_i = -L_0(1 - 0.001S_i) + T_i c_i \tag{2}$$

where S_i is the bulk sea ice salinity (psu). Finally, for the BP case, we assume that (i) the freezing point of seawater [1] is a linear function of salinity $T_f = -\mu S$, where $\mu = 0.054$°/psu, (ii) the specific heat of the brine c_w is constant, and (iii) the brine is always at the freezing point for its salinity (generally higher than S_i). In that case, the brine fraction is $\alpha = -\mu S_i/T_i$ and the energy is

$$E_i = -L_0(1-\alpha) + c_i(1-\alpha)T_i + c_w\alpha T_i = -L_0(1+\mu S_i/T_i) + c_i(T_i + \mu S_i) - c_w\mu S_i \tag{3}$$

The first term is the latent heat of the ice fraction. The second and third terms are the enthalpy of the ice and brine respectively.

Because the freezing temperature of seawater depends on salinity, sea ice and seawater can coexist and phase changes can occur over a range of temperatures. Given that the energy of sea ice defined above depends on temperature and sea ice salinity, the amount of energy required to change phase will vary. A phase change may occur in combination with a temperature change, and so we must account for both latent and sensible heat in cooling seawater to freezing and then freezing it, or in warming sea ice to melting and then melting it.

In general, a process that converts water at T_w and S_w to ice at T_i and S_i (or vice versa) releases (or requires) energy equal to $E_o(T_w, S_w) - E_i(T_i, S_i)$ where E_o is the energy of the seawater (J/kg). For our

[1] The freezing point of salt water is an almost linear function of salinity S, $T_f(S) = -0.0575S - 0.0002154996S^2 + 0.001710523S^{3/2}$ (Fofonoff and Millard, 1983). It greatly simplifies some of the ice thermodynamic calculations if this is assumed to actually be linear (the difference from the more complicated dependence is small). There is a substantial pressure dependence though, and this can be an important factor in the subsurface ocean $T_f(S,P) = T_f(S) - 7.53\times10^{-8}P$ (P is the gauge pressure in Pa).

purposes, we assume that the specific heat of seawater is constant over the small range of temperatures and salinities relevant for ice–ocean interfaces, and hence $E_o(T_w) = T_w c_w$. If the energy of the ocean component is defined using a variable specific heat (for instance if potential enthalpy is used as the prognostic variable, rather than potential temperature (e.g. Russell et al., 1995)), the formula is slightly altered. There is a minor inconsistency when adding brine from the ice to the ocean in such cases since in order to conserve energy, the effective temperature for the brine "in the ice", will differ from the temperature of the brine "as seawater" by the ratio of the constant specific heat used in the sea ice model to the actual specific heat, but this is a very small percentage error.

Clearly, if $T_w = T_i$, the energy released is an effective latent heat (the energy required to change phase at constant temperature), which in general will differ from the latent heat of pure ice at 0 °C (L_0). Even for pure ice, the effective latent heat of melting must depend on the difference of the specific heats of the liquid and solid phases e.g. $L_0 + T(c_w - c_i)$, as can be seen from considering how to conserve energy in a melt/cool/freeze/warm cycle. Only if both specific heats are neglected (as they are for instance for water vapour and liquid in some atmospheric models) will the temperature dependent term be zero. It is therefore necessary for the ocean to know the appropriate definition of the ice energy so that energy changes due to ice formation within the ocean can be consistently made in each component (this is discussed in more detail in Section 3). Depending on the formulation (and the ice temperature), the neglect of the temperature dependence is a 1–10% error in the energy.

The boundary conditions we derive will be appropriate for the most realistic cases (full exchange of freshwater, salt and energy between the ice and ocean, a salinity budget for the sea ice etc.), but we note where the effect of commonly-used simplifications would make a difference. The impact of choosing a different formulation (i.e. the difference between PI and BP) is likely to be more important than making any one formulation energy-conserving, but even these changes can be significant. For instance, Bitz and Lipscomb (1999) found a 10–20% changes in the ice thickness when fixing conservation problems associated with brine pockets in the Semtner 3-layer scheme. While the most important fluxes are of fresh water, salt and energy, we also consider the boundary conditions governing other passive tracers (e.g. particles, dissolved substances, water isotopes, 'age', 'colour' etc.) since these are increasingly being incorporated into earth system models.

We will discuss a number of parameterized processes at the ice–ocean interface. While the form of the parameterized fluxes is generally empirical (and therefore uncertain to a significant degree), we will focus on the need to make the formulations consistent, regardless of the exact parameter values chosen. The discussion is broken into five main sections. The first deals with an improved formulation for the fluxes at the base of the ice, and the second deals with the implications of energy conservation on oceanic frazil ice production. For completeness, we discuss lateral fluxes at the sea ice edge, and some issues related to snow–ice formation in the next two sections. Finally, boundary conditions and problems relating to the ice dynamics and the ocean free surface are discussed in Section 6.

2. Basal ice–ocean fluxes

Observations of basal sea ice conditions reveal a highly complex topography of ridges and keels with complex turbulent motions at all scales. However, it appears that the fluxes between the ice and ocean mixed layer are principally governed by the very thin viscous boundary layer immediately next to the ice (Mellor et al., 1986; McPhee et al., 1987). Gradients of temperature and salinity are greatest across this interface, and we therefore assume that away from this interface, the ocean conditions can be considered well mixed. The boundary conditions then need to relate the fluxes to the basal ice conditions and ocean mixed layer. One consequence of this physical environment is that ice often persists in water that is measurably warmer than its freezing point, as is frequently observed. In formulations based on the 'ice-bath' assumption, any excess energy in the ocean mixed layer is used to melt ice, leading to enhanced melting in the spring/summer, and early freeze-up in the fall/autumn (Fichefet et al., 1998; Holland and Jenkins, 1999). Improving this aspect of coupled simulations is the principle goal of this section.

Many formulations have assumed that the ocean is able to specify the temperature at the ice–ocean interface. However, in general, this will be a function of the ice melt/formation rate and is not a priori determinable. We therefore subsume the calculation of the boundary properties into the boundary conditions themselves (following McPhee et al., 1987; Holland and Jenkins, 1999). The 'ice-bath' formulation can however be considered as a limiting case (at high ocean turbulence).

The conditions at the boundary are a function of the diffusive (heat) flux into the ice, the turbulent fluxes from the ocean mixed layer, and the melt or ice formation rate. All of these fluxes are a function of the boundary values of temperature and salinity (T_b, S_b). Continuity at the interface implies that T_b is at the freezing point for water with the boundary salinity, S_b. Given the extremely small heat capacity and mass of this boundary layer, it is convenient to assume that they are actually zero, and then set the boundary values using a 'flux-in equals flux-out' approximation. As an aside, we note that a similar assumption at the atmosphere–ice boundary can be more complicated since many atmospheric models make the same assumption for calculating the surface air temperature. We neglect the impact of solar radiation in the viscous sublayer, although it is an important energy flux into the mixed layer.

The upward diffusive heat flux $-\lambda(T_i, S_i)\mathrm{d}T_i/\mathrm{d}z$ is evaluated at the base of the ice. The diffusion coefficient λ can be a function of temperature and salinity (independent of other thermodynamic considerations involving salt) and the ice temperature gradient can be estimated as $\mathrm{d}T_i/\mathrm{d}z = (T_i - T_b)/\Delta h$, where Δh is the thickness of ice from the base to where the lowest ice temperature above the base is defined. This term is best determined implicitly to avoid time stepping constraints when the ice is thin.

The turbulent fluxes from the ocean mixed layer are governed by a complicated set of equations (McPhee et al., 1987) depending on the input of turbulent kinetic energy, the stability and the differing molecular viscosities for salt and heat. Each flux can be written as $\rho_w \gamma (X_b - X_o)$, where γ (m/s) is the relevant turbulent exchange velocity, ρ_w the ocean density, and X_b, X_o the basal and ocean mixed layer values for any particular tracer (temperature, salinity or concentration). Following Holland and Jenkins (1999), the heat flux can be estimated using a 1-, 2- or 3-equation approach depending on assumptions about the boundary temperature and salinity. The 1-equation approach simply fixes the boundary temperature to a constant (i.e. −1.8 °C). In the 2-equation approach, the boundary salinity is assumed equal to the mixed layer value and is equivalent to assuming that the turbulent exchange coefficient for salinity is significantly larger than that for heat. However, theoretical considerations and observations imply that the opposite is actually true. Therefore we discuss the more general 3-equation formulation where the boundary salinity is determined as a function of melt rate and ocean turbulent flux.

The equations that must be satisfied at the interface are

$$T_b = -\mu S_b \tag{4}$$

$$-\lambda \frac{(T_i - T_b)}{\Delta h} + \rho_w c_w \gamma_T (T_b - T_o) = -F_m(E_o(T_b, S_b) - E_i(T_{ib}, S_{ib})) \tag{5}$$

$$\rho_w \gamma_S (S_b - S_o) = -F_m(S_b - S_{ib}) \tag{6}$$

where subscripts o, b, i and ib denote the ocean mixed layer, the boundary values, the ice values and the value for the mass being transferred, respectively. The properties T_{ib}, S_{ib} of any melt or new ice, will depend on the sign of the melt rate F_m (kg/m^2/s) (negative values denote ice formation),

$$S_{ib} = S_i, \;\; T_{ib} = T_i \quad F_m > 0, \quad \text{or} \quad S_{ib} = f_S S_b, \;\; T_{ib} = T_b \quad F_m < 0 \tag{7}$$

where f_S is the fraction of the boundary salinity that is initially retained within the ice. In reality f_S can be relatively large (up to 0.35 or so, corresponding to a salinity of 13 psu for ice derived from 35 psu seawater). Brine drainage reduces the ice salinity over time, but if this process is not considered within the ice model a fixed value of 0.14 (giving a sea ice salinity of 5 psu) is appropriate. We do not consider brine drainage as a direct input into the boundary equations, although that might be considered in future extensions. Eqs. (4)–(7) differ from those used in Holland and Jenkins (1999) since we incorporate the temperature and salinity dependence of the internal energy and an upstream scheme for the salt and heat content of the mass flux. Note that these conditions are perfectly conserving and include the 'meltwater advection' terms (the internal energy of the meltwater) that have sometimes been neglected (Jenkins et al., 2001). The actual (downward) fluxes between the ice and ocean components of heat (F_H, W/m^2) and salt (F_S, kg/m^2/s) are then defined as

$$F_H = \lambda(T_i - T_b)/\Delta h + F_m E_i(T_{ib}, S_{ib}) \quad \text{or,} \tag{8a}$$

$$= \rho_w c_w \gamma_T (T_b - T_o) + F_m E_o(T_b, S_b) \tag{8b}$$

$$F_S = 0.001 F_m S_{ib} \tag{8c}$$

The 0.001 factor in F_S simply converts psu to kg/kg.

The tracer equations are assumed to be analogous to the salinity (i.e. we use γ_S for the tracer exchange velocity), and must satisfy

$$\rho_w \gamma_S (X_b - X_o) = -F_m(X_b - X_{ib})$$

with

$$X_{ib} = X_i, \quad F_m > 0, \quad \text{or} \quad X_{ib} = f_X X_b, \quad F_m < 0$$

where f_X is ratio of the amount in new ice to the boundary tracer amount. This could be affected by solute rejection, or fractionation of isotopes for instance. The net downward flux is $F_X = F_m X_{ib}$.

It remains to determine the turbulent exchange velocities γ_T, γ_S. As the ice–ocean stress increases, so will the turbulent mixing, leading to a greater flux towards the ice and diminishing the gradients across the boundary layer, and so a dependence on $u^* = \sqrt{(|\tau|/\rho_w)}$ (m/s), the friction speed derived from the ice–ocean stress, is clearly indicated. This can be a simple linear function, or a more complicated expression that depends on the stability at the interface. The simplest expression has $\gamma_T = 9 \times 10^{-3} u^*$ and $\gamma_S = 0.025\gamma_T$ (M. McPhee, pers. communication). For situations such as for lakes with complete ice cover and where there is no tidal or convective mixing, small values of $\gamma_T = 1 \times 10^{-7}$ m/s and $\gamma_S = 3 \times 10^{-9}$ m/s (for tracers) are reasonable (Liston and Hall, 1995).

A more involved calculation (McPhee et al., 1987; Holland and Jenkins, 1999) has $\gamma = u^*/(\Gamma_{\text{turb}} + \Gamma_{\text{mole}})$, where Γ_{turb} is the same for all fluxes, but Γ_{mole} depends on the molecular viscosity for that tracer, i.e. $\Gamma_{\text{mole}} = 12.5X^{2/3} - 6.0$ where X is either Pr or Sc (the Prantdl and Schmidt (no relation) numbers) for heat and salt respectively. For heat, $Pr = 13.8$ and $\Gamma_{T\,\text{mole}} = 65.9$, and for salt, $Sc = 2432$ and $\Gamma_{S\,\text{mole}} = 2255$. The turbulent component can be written

$$\Gamma_{\text{turb}} = (1/\kappa)(\log(u^{*2}\zeta\eta^2/5fv) - 1) + 1/(2\zeta\eta)$$

where $\kappa = 0.4$ is the Von Karman constant, $\zeta = 0.052$ an empirical constant, $v = 1.95 \times 10^{-6}$ m^2/s is the kinematic viscosity, f the Coriolis parameter and η is the stability parameter. η can be expressed in terms of the buoyancy flux, but for simplicity we will assume that $\eta = 1$, simplifying the above expression to leave

$$\Gamma_{\text{turb}} = 2.5\log(5300u^{*2}/f) + 7.12$$

Putting it together gives, for typical values of $u^* = 0.01$ m/s, $\gamma_T = 1.2 \times 10^{-4}$ m/s, $\gamma_S = 4.4 \times 10^{-6}$ m/s, slightly larger than the simplest expressions given above.

In general, Eqs. (4)–(7) cannot be solved directly, and so we use the Newton–Raphson method to converge quadratically (within five iterations) to a solution. We define a function $f(S) = S - S_b(S)$, which is the difference between an initial guess of the boundary salinity, and the value that arises from solving Eqs. (4)–(7). Specifically, we assume an initial value of S_{b0}, determine T_b from (4), determine the sign of F_m from (5), the properties of the melt or new ice from (6), the value of F_m from (5) and then determine a new value of S_b from (6). This defines the function f, whose derivative with respect to S_{b0} is also easily calculated. Newton's method is then used to refine the estimate of S_b and the iteration continues. We include code that performs this calculation as supplementary material to this paper.

With no salinity effects in either the boundary temperatures or sea ice (i.e. $S_b = S_i = S_{ib} = 0$), the equations can be solved directly, although an iteration is still necessary for the case of complete brine rejection over a salty ocean ($S_b \neq 0, S_i = S_{ib} = 0$). If the boundary salinity is assumed to be that of the mixed layer (2-equation formulation), $S_b \equiv S_o$, Eq. (6) is ignored, and γ_T should be smaller ($\approx 6 \times 10^{-3}$ m/s) to account for the slight difference in the boundary temperature. In the limit of strong ocean turbulence ($\gamma_T, \gamma_S \to \infty$), the boundary values are identical to the mixed layer values, and the ocean mixed layer must be at the local freezing point. Currently, GISS uses the full 3-equation form, while CCSM assumes $S_b \equiv S_o$ and $T_b = -1.8$ °C (1-equation formulation), and MPI assumes γ_T, $\gamma_S \to \infty$ (the ice-bath formulation).

The difference made by having the correct righthand side in Eq. (5) (as opposed to the commonly used $-F_m L_0$) is on the order of a few percent for the PI and SI cases, but can lead to a 40% or so error in the BP formulation when freezing occurs. The meltwater internal energy term in the heat flux can be up to 5% of the total. Fig. 1 shows an example calculation demonstrating the effect of different ice energy (PI and BP: SI is very similar to PI and is not shown for clarity) and basal flux formulations. BP always has more ice formation for a given heat flux, and both the 2- and 3-equation formulations require a greater u^* to initiate melting (i.e. ice will persist longer in those cases) compared to the simple 1-equation case. The 3-equation case has an intermediate

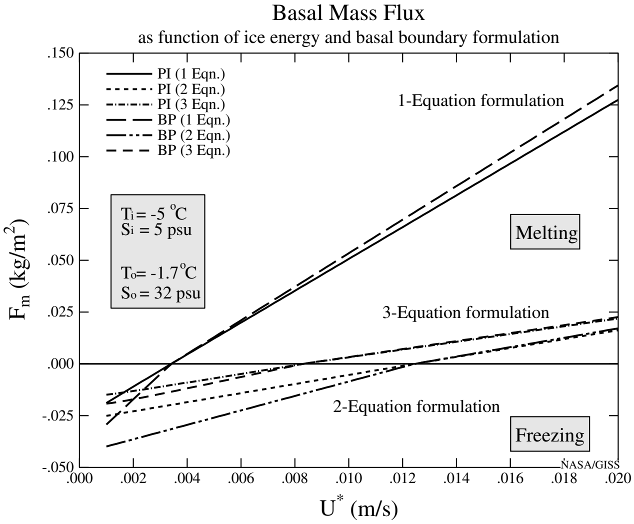

Fig. 1. An example calculation of the basal mass flux as a function of ice energy (PI or BP) and basal boundary condition. The ice temperature and salinity are fixed at −5 °C and 5 psu respectively, and the ocean temperature and salinity are −1.7 °C and 32 psu. These values were chosen to illustrate the threshold of ice formation/ice melt being crossed as u^* increases. The upper lines use the simplest 1-equation formulation (where the assumed basal temperature is a constant −1.8 °C, $\gamma_T = 0.006u^*$), the bottom lines use a 2-equation formulation (assuming that the basal temperature is the freezing point at the ocean salinity, $\gamma_T = 0.006u^*$), and the middle lines a 3-equation formulation as discussed in Section 2 ($\gamma_T = 0.009u^*$, $\gamma_S = 0.025\gamma_T$).

melt/freeze point compared to the other formulations, but a significantly smaller rate of change of ice formation as u^* increases. The difference between PI and BP is larger near the ice melting point, which is why there is more divergence in the ice formation regime (at the freezing point of seawater) compared to the ice melting regime (at −5 °C in this example).

Interior and surface melt also need to be considered carefully. Pure ice melts at 0 °C and by definition, its runoff has zero energy. However, for the BP case melting can occur below 0 °C and therefore the energy of the melt will be negative and needs to be added to the ocean.

3. Frazil ice formation

As a matter of principle, the ice formation rate in the open ocean cannot be specified by consideration of the surface conditions only. For instance, in cases where the mixed layer extends more than one grid box down, freezing may occur at lower boxes, and the resulting sea ice may have different properties, due to the pressure dependence of the freezing temperature, and possibly different salinities. In addition, any inclusion of glacial or iceberg melting may produce supercooled water at depths of a few hundred meters which can subsequently freeze (producing 'marine' ice (Grosfeld et al., 1998)).

Thus, if the frazil ice formation is calculated within the sea ice component (or special flux module) possibly the whole column hydrography needs to be passed from the ocean model.

Alternatively, the ocean model can compute frazil ice formation, but it needs to know the sea ice energy definition. This leads to problems for the second principle outlined in the Introduction, that separate model components should not assume anything about the others. In practice, this complexity has been dealt with either by assuming that only surface conditions are important (MPI), or by ensuring that the sea ice energy definitions are consistent across models (CCSM, GISS) (for example, CCSM assumes that all ice forms at −1.8 °C, with a salinity of 5 psu, and hence E_i is predetermined). We therefore recommend that if all possible modes of ice formation are to be allowed for, the ocean model must use generalised code that calls a utility function from the ice model for the energy of sea ice.

For any grid box within the ocean, the amount of ice formation will be calculated based on the energy deficit $\Delta E = E_o - E_f$ (J/kg) of the box compared to a box at the local freezing point (where $E_f = E_o(T_f(S,P),S)$ is a function of salinity and gauge pressure). Assuming that total mass and energy are conserved when an amount of ice is formed leads to

$$E_o m_o = E_f(m_o - m_i) + E_i(T_f, S_i)m_i$$

where m_i (kg/m^2) is the ice mass of salinity S_i formed from the original m_o (kg/m^2) mass of the ocean box, and $E_i(T,S)$ is defined by the ice model following the formulations discussed in the Introduction. Rearranging we get

$$m_i/m_o = -\Delta E/(E_f - E_i(T_f, S_i)) \tag{9}$$

where m_i/m_o is the mass fraction of the box that is frozen. The denominator is exactly the effective latent heat at the freezing point of the ocean defined in the Introduction. Substituting in and assuming a constant specific heat (although that is not strictly required) we get

$$m_i/m_o = \Delta E/(-L_0 + T_f(c_i - c_w)) \tag{PI}$$

$$m_i/m_o = \Delta E/(-L_0(1 - 0.001S_i) + T_f(c_i - c_w)) \tag{SI}$$

$$m_i/m_o = \Delta E/(-L_0(1 + \mu S_i/T_f) + (T_f + \mu S_i)(c_i - c_w)) \tag{BP}$$

for the three different ice energy formulations.

As noted above, there may be a small inconsistency in assuming that the specific heat of seawater is a function of temperature and salinity, while the specific heat of brine is constant. As long as the calculations clearly separate the ice energy calculation from the ocean energy as in Eq. (9), there is no problem. Incorporating the variation of specific heat within the ice model could be done, but it is a relatively small term.

4. Lateral fluxes

Open water production by lateral melt on the kilometer scale is significant primarily in the marginal ice zone, where ice can be advected into warm ocean water and vice versa. Sea ice models often purposefully overestimate lateral melt to compensate for their failure to resolve first year ice, which would melt away owing to top and bottom ablation during the melt season. Common strategies have been to either assign a fraction of the basal heat flux to the lateral flux or to assume a linear thickness distribution and reduce the ice area accordingly when there is melt at the top or bottom surfaces (as in the MPI model, and previous versions of the GISS model). However, if better estimates of the basal flux (as discussed above) are to be used, a separate formulation of the lateral fluxes is generally necessary. A subgrid-scale parameterization of the ice-thickness distribution resolves thin ice explicitly and eliminates the need for ascribing an unrealistically high fraction of the ocean–ice heat flux toward lateral melt. This offers the opportunity to use a more physically based parameterization of the lateral heat flux, as described here based on the CCSM coding (Briegleb et al., 2002).

The lateral heat flux depends on the floe geometry and the interfacial receding rate:

$$F_{\mathrm{lat}} = -(E_{\mathrm{i}}m_{\mathrm{i}} + E_{\mathrm{s}}m_{\mathrm{s}})M_{\mathrm{a}}p$$

where E_{i} and E_{s} are the vertically averaged energies of the sea ice and snow, m_{i} and m_{s} are the mass per unit area of ice and snow, M_{a} is the interfacial melting rate, and p is the perimeter of the interface per unit area. We assume that the entire vertical column of ice and snow is in contact with the ocean and that melting occurs at a uniform rate over the lateral interface. A maximum amount of melting is given by the available heat for melting in the ocean mixed layer.

The interfacial melting rate is based on an empirical expression from ablation data taken during the Marginal Ice Zone Experiment by Maykut and Perovitch (1987). They found $M_{\mathrm{a}} = m_1(T_{\mathrm{l}} - T_{\mathrm{i}})^{m_2}$, where $m_1 = 3\times10^{-6}\ \mathrm{m\,s^{-1}}\ (^{\circ}\mathrm{C})^{-m_2}$ and $m_2 = 1.36$ are best fit estimates, T_{l} is the lead temperature, and T_{i} is the temperature at the lateral interface. Ideally T_{i} should be computed from a procedure similar to the basal flux calculation. However, due to uncertainty in the other parameters, particularly the ice perimeter and lead temperature, the complexity is unwarranted and we let $T_{\mathrm{i}} = -\mu S_{\mathrm{o}}$, the freezing temperature of the ocean surface. The perimeter of the lead-ice interface p, depends on the floe distribution and geometry, however this is both poorly observed and difficult to resolve in models. Observational estimates of the floe-size distribution span many orders of magnitude (e.g. Holt and Martin, 2001), but Steele (1992) argued that lateral melt is only significant when floes are fairly small, or $p \approx 10^{-3}\ \mathrm{m}^{-1}$. CCSM and GISS use a value $p = 4.8\times10^{-3}\ \mathrm{m}^{-1}$, but this should probably be considered a tunable parameter.

Observations from SHEBA demonstrated that during the melt season, very strong stratification can build up in leads in calm conditions. Temperatures in the leads can exceed the local freezing point by up to a couple of degrees, clearly affecting the lateral melt rate. At present, none of the ocean models considered here incorporate a separate calculation of the open-water sea surface temperature although this is being explored in recent research (Holland, 2003). Therefore for simplicity, the lead temperature is usually taken as the uppermost layer temperature (T_{o}).

5. Snow–ice formation

Heavy snow conditions (particularly in the southern hemisphere) can push the snow–ice interface below sea level, causing seawater to flood the snow. Observations show that the flooded layer freezes in time into a high salinity layer. Introducing a liquid layer in between the ice and snow is quite complicated numerically (Saloranta, 2000) and can be avoided, albeit crudely, by assuming the flooded seawater freezes instantly (Leppäranta, 1983, 1993). The mass of seawater that floods and the amount of snow that compresses to ice, are determined by the amount of latent heat that can be absorbed by the snow, and the need to restore the snow–ice interface to the ocean surface. Two extreme cases can be easily examined: (i) no seawater mass is added, and snow is compressed to an amount of new ice equal to the initial depression below the water line; and (ii) seawater floods a layer and freezes but the total height of snow and ice does not change. The first case is simple and easy to implement (but is not very realistic), while the second is closer to reality, but requires that the snow being flooded is cold enough to freeze that mass of seawater. Between the two extreme cases, smaller amounts of seawater flooding can be acceptable, providing that more snow is compressed to compensate. In case (i) more snow is compressed than is necessary to return the snow–ice interface to sea level in a given time-step, and over the course of a year, the amount of ice gained by snow–ice conversion is less than it would be if seawater were allowed to freeze.

Snow–ice formation occurs when

$$m_s > m_i \frac{\rho_w - \rho_i}{\rho_i}$$

where m_s, m_i are the mass of snow and ice (kg/m^2), and ρ_i, ρ_w are the ice and seawater density. The depth to which the water line is above the snow–ice interface is $z_0 = (m_i + m_s)/\rho_w - m_i/\rho_i$. In case (i) where no seawater mass is added, the mass of snow that needs to be compressed to ice is $z_0\rho_i$, which implies a reduction in snow thickness by $z_0\rho_i/\rho_s$ where ρ_s is the snow density. CCSM uses this prescription, but since the snow is fresh an additional amount of salt is added equal to $0.001S_{ref}z_0\rho_i$ where S_{ref} is the reference sea ice salinity. The energy of the newly formed sea ice layer is equal to that of the snow, which necessarily makes the temperature of the layer somewhat colder than the snow it originated from if $S_i > 0$. However, the layer is usually very thin, so it has a negligible effect on the sea ice temperature profile over time.

If an amount of seawater m_w kg/m^2, is allowed to freeze depending on the capacity of the snow to absorb the latent heat, the amount of snow that needs to be compressed (Δm_s) must satisfy

$$\Delta m_s = z_0\rho_i - m_w \frac{\rho_w - \rho_i}{\rho_w} \tag{10}$$

with z_0 defined as above. The maximum amount of seawater flooding (corresponding to case (ii)) is

$$m_w = z_0\rho_w \frac{\rho_i - \rho_s}{\rho_w + \rho_s - \rho_i} \tag{11}$$

but the actual amount of freezing is limited by the energy consideration, i.e.

$$m_w < \Delta m_s \frac{E_s - E_i(T_f(S_w), S_i)}{E_i(T_f(S_w), S_i) - E_o} \tag{12}$$

where $E_s = -L_0 + T_s c_i$ is the initial snow energy (at temperature T_s) and E_o is the initial enthalpy (J/kg) of the seawater. $E_i(T_f(S_w), S_i)$ is the maximum energy in the newly formed snow–ice (that froze at the freezing point of the seawater) and now has a salinity of S_i (either predetermined or calculated as in Eq. (7)). Combining Eqs. (11) and (12) then determines the amount of seawater freezing possible. Generally, allowing seawater to freeze in such cases can increase the amount of snow–ice formation by up to a factor of 2.5. Currently, neither the GISS nor MPI models include this physics.

6. Ocean–ice dynamic interactions

The full interaction of the sea ice with ocean dynamics (and vice versa), implies that the ocean model 'feels' the ice pressure and stress and that the ice 'feels' the sea surface height and ocean currents. This has only rarely been considered in the context of fully coupled models due to the frequent assumption of an ocean rigid lid. However, with the increasing use of free surface formulations there are a number of problems that can emerge.

Firstly, the dynamical boundary conditions for the ocean require, in principle, that the pressure at the surface of the ocean is known. This pressure consists of the anomalous atmospheric pressure, and also the integrated pressure of the sea ice. This can lead to variations of the sea surface height that are quite significant in sea ice regions. Consequently, it is important that the integrated column pressure in the ocean does not change as a function of sea ice formation (i.e. any mass lost from the ocean due to ice formation must appear in the surface pressure condition). With a z-coordinate model, the depth of of the first layer is often fixed (typically at around 10 m), however the variations in sea surface height associated with conceivable sea ice variations are of the same order of magnitude. Thus, there is potentially a (numerical) problem of pushing down the sea surface height below the level of the first grid box. In the GISS ocean model (Russell et al., 1995, 2000), the vertical coordinate is sigma-like at each grid point, but with varying numbers of levels dependent on the ocean depth so that it resembles a z-coordinate model. Thus the mean depths of the grid box levels follow the surface height down, neatly avoiding this potential problem, at the cost of only minor extra complexity in the dynamics.

A second problem arises when the sea ice dynamics are fully coupled to the ocean surface conditions (including the sea surface height). The ice momentum equation includes forcing from the atmosphere–ice and ocean–ice stresses, and the sea surface height gradient. Note that the sea surface height is the height that would be observed in the ocean after any displacement by ice. Since the diagnosed sea surface height from ocean models does not generally include the displacement term, the effective sea surface height needs to have an additional m_i/ρ_w where m_i is the total mass of sea ice and snow in the box (kg/m^2). Without this term the sea surface tilt will be too large and will lead to a unrealistic drift of thin ice towards thick ice. The sea surface height field can be highly variable due to the surface gravity–wave field and noise from the ocean dynamics, and this variability has the potential to produce an ocean–ice dynamical instability.

Instabilities have been observed in a number of coupled models that have included both free surface and fully coupled ice dynamics (GISS, MPI and GFDL). Grid-point noise in the ocean dynamics can give rise to an up–down–up pattern of sea surface height variations. Without the effects of sea ice, this mode usually remains bounded. When sea ice is present, this pattern gives rise to a convergent–divergent pattern in the ice velocities that can reinforce the sea surface height variations, amplifying the pattern. The instability occurs primarily because ice and ocean dynamics react separately to the pattern in a 'constructive' way.

Two solutions have been found to remove this problem while maintaining full coupling (the sea surface height forcing could always be disabled otherwise). For the GISS model, we found that smoothing the ocean height field in time (i.e. only passing the average of the current and past time step sea surface height) removed the problem entirely. In the MPI model, sea level (in the ocean), ocean and ice velocities ($\mathbf{u}_i$) are calculated implicitly, whereas tracer and ice advection is done with an explicit scheme. The sea ice advection directly affects sea level due to the divergence of mass fluxes. Replacing the sea level η (defined in the ice free parts of the box) in the implicit solution of the momentum balance equation for ice by

$$\eta + \delta t \nabla \cdot (m_i \mathbf{u}_i)/\rho_w$$

solved the problem. Practically, it is important to use the same discretisation and advection scheme for the calculation of the divergence as for the later advection of sea ice. NCAR CCSM has not yet experienced similar problems since they assume no mass exchange between ice and ocean (see Section 7) and do not allow the sea ice mass to affect the ocean surface pressure.

7. A simplifying assumption: no mass exchange between ice and ocean

For a number of reasons (e.g. rigid lid in the ocean), it may be convenient to disallow mass exchanges between the ice and ocean models (although a salt flux equivalent to the freshwater flux needs to be included to model brine rejection effects). However, the conservation of energy implies that the energy fluxes that would be accompanied by such mass fluxes need to be included regardless of whether mass is properly conserved. The terms involving the latent heat are large and those involving the specific heat portions are likely to be small, but it is not onerous to include these as well. CCSM makes this assumption and, since the mass of melted ice is not fluxed, is also free to set the heat capacity of the melt to zero. This is equivalent to dropping the last term in Eq. (3) (Bitz and Lipscomb, 1999). As discussed above, disallowing mass exchanges between the components implies that the ice pressure cannot influence the ocean momentum, and thus the instability in Section 6 is avoided (at the cost of non-conservation of freshwater and salt).

8. Summary and conclusions

We have discussed a number of different processes, not all of which will be included in any particular climate model. However, regardless of the complexity of the simulated physics, the principles discussed here should still be applicable and useful in ensuring conservation. In order for existing sea ice and ocean components used in coupled models to satisfy the conservation criteria in the most general of circumstances, we make a number of recommendations:

1. A clear definition of energy $E_i(T_i, S_i)$ for the ice model is required. This should be contained within a function accessible from outside the ice model.
2. This energy should be used in the basal ice flux conditions (Eq. (5)) and for frazil ice production in the ocean model (Section 3). This correctly deals with the temperature (and possibly salinity) dependence of the effective latent heat.
3. The internal energy associated with any mass transfers (i.e. meltwater/frazil ice production) should be included in the energy fluxes, even those related to mass fluxes that for other reasons may be neglected in the mass budget, i.e. Eq. (8) should be used for the ice–ocean heat flux.
4. The 3-equation basal flux formulation presented here can make a significant difference of ice melt rates (Fig. 1) and is not difficult to implement, regardless of the ice model used. A subroutine for this calculation is included in the online supplementary material accompanying this paper.

5. A separate lateral melt parameterization is generally required if an improved basal flux formation is included, and a straightforward example is described in Section 4.
6. A snow–ice formation parameterization can easily be incorporated (although the effects in coupled models are not yet fully quantified).
7. Full interaction of the sea ice and ocean dynamics is desirable but can be problematic. Practical solutions for dealing with large sea surface height variations and potential instabilities do however exist.

Implementation of these suggestions will have varying effects. Choosing a different ice model formulation (PI vs. BP for instance), or going from a 1-equation to a 3-equation basal heat flux calculation (item 4) will have more effect than making any particular formulation mass and energy conserving (items 2 and 3 above). However, the latter can change fluxes by up to 40% (in the BP case), although in a coupled model compensating feedbacks may reduce the magnitude of the effect on the climatology. The sensitivity of fully coupled climate simulations to these items will likely depend on the model and will be quantified in future work.

A related issue to those discussed here is the definition of the buoyancy forcing B (m^2/s^3) at the ocean surface. This is often an important term in calculations of upper ocean mixing (for instance in the K-profile parameterization (Large et al., 1994)). When salt and freshwater fluxes are being added as well as heat, the expression for the buoyancy forcing must be altered to take account of possible dilution. The real buoyancy forcing can be specified independently of what is actually added to the ocean as

$$B = -\frac{g}{\rho_w}\left(\frac{\alpha}{c_w}F_H - \beta F_S - (\alpha T - \beta S)F_m\right)$$

where α, β are the thermal and saline expansion coefficients and F_m ($kg/m^2/s$), F_H (W/m^2) and F_S ($kg/m^2/s$) are the downward mass, heat and salt fluxes respectively (defined in Eq. (8)). The value of this expression can be significantly different from the actual change in buoyancy if, for instance, mass fluxes are not exchanged, or the freshwater flux is converted to an equivalent salt flux. In line with our comments concerning energy fluxes, we feel that it is appropriate to use the real forcing, rather than the approximate value set by the simplifications in any model component.

We have presented a summary of best current practice for coupling ice and ocean models in way that we hope will be useful for other modelers working with similar issues. We re-iterate the importance of full energy, mass and salt conservation in improving the interoperability of climate model components and eliminating possible systematic energy biases related to sea ice processes.

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On p. 69 of Schmidt et al (2004), Equ. 12 should have defined the limit on the actual amount of freezing as

$$m_w < \Delta m_s \frac{E_s - E_i(T_f(S_w), 0)}{E_i(T_f(S_w), S_i) - E_o} \tag{12}$$